NATIONAL CENTER
FOR COMPUTATIONAL SCIENCES

NCCS High-Performance Computing Allocations for FY 2006

Both Cray machines—Phoenix (X1E) and Jaguar (XT3)—will be used to complete simulations in weeks instead of months or years needed for other high-performance computing systems.

On December 19, allocations were made for the leadership computing resources of the National Center for Computational Sciences (NCCS), located at Oak Ridge National Laboratory (ORNL). A total of 17 projects were awarded to researchers across the country, representing nearly 90% of the available NCCS leadership computing resources. The call for proposals issued by the U.S. Department of Energy (DOE) was to promote computationally intensive, grand-challenge scale research projects. This year's research topics range from exploration of causes of the collapse of supernovae to predicting future climates that result from human actions. Further, new models for the design of fusion reactors and high-energy accelerators will be developed through unique studies only possible on the computational resources of the NCCS. A complete list of the projects can be seen at http://www.nccs.gov/leadership/projects/fy06.html.

"Advanced scientific computing is critical to DOE's missions," said U.S. Department of Energy Secretary Bodman. "Scientific computing is essential to simulating and predicting the behavior of nuclear weapons and accelerating the development of new energy technologies." The impact of research at the NCCS can be realized in two ways. First, projects using the high-performance computing capabilities at the NCCS will take advantage of the fast processing speed of computers such as the Cray X1E. Second, another Cray—the XT3 system and the newest addition to the NCCS—offers balanced massively parallel processing architecture to run large, complex applications across hundreds or even thousands of processors.

Scientists from ten research facilities and universities as well as ORNL scientists are leading these 17 projects. Many projects are composed of multidisciplinary teams that seek answers to complex problems. For example, a team modeling the core collapse of a supernova comprises specialists from fields of nuclear and astrophysics, applied mathematics, and general relativity. A team project such as this is called an "end station" project because it provides a centralized place where researchers can develop code to benefit the related research community. Other projects focus more on single research areas. A mix of both types of projects will be running throughout the year; these along with their principal investigators are listed here.

- **Monte Carlo Simulation and Reconstruction of CompHEP–produced Hadronic Backgrounds to the Higgs Boson Diphoton Decay in Weak-Boson Fusion Production Mode**
  Harvey Newman (California Institute of Technology)
- **The Role of Eddies in the Thermohaline Circulation**
  Paola Cessi (Scripps Institution of Oceanography, UCSD, CA)
- **Ignition and Flame Propagation in Type Ia Supernovae**
  Stan Woosley (University of California, Santa Cruz)

- **High-Fidelity Numerical Simulations of Turbulent Combustion – Fundamental Science Towards Predictive Models**
  Jackie Chen (Sandia National Laboratories)
- **Climate-Science Computational End Station Development and Grand Challenge Team**
  Warren Washington (National Center for Atmospheric Research)
- **Ab-initio Nuclear Structure Computations**
  David J. Dean (Oak Ridge National Laboratory)
- **Performance Evaluation and Analysis Consortium (PEAC) End Station**
  Patrick H. Worley (Oak Ridge National Laboratory)
- **Computational Design of the Low-loss Accelerating Cavity for the ILC**
  Kwok Ko (Stanford Linear Accelerator Center)
- **Gyrokinetic Plasma Simulation**
  W. W. Lee (Princeton Plasma Physics Laboratory)
- **Exploring Advanced Tokamak Operating Regimes Using Comprehensive GYRO Gyrokinetic Simulations**
  Jeff Candy (General Atomics)
- **Multi-dimensional Simulations of Core-Collapse Supernovae**
  Anthony Mezzacappa (Oak Ridge National Laboratory)
- **Multi-dimensional Simulations of Core-Collapse Supernovae**
  Adam Burrows (University of Arizona)
- **Simulation of Wave-Plasma Interaction and Extended MHD in Fusion Systems**
  D. B. Batchelor (Oak Ridge National Laboratory)
- **Eulerian and Lagrangian Studies of Turbulent Transport in the Global Ocean**
  Synte Peacock (University of Chicago)
- **An Integrated Approach to the Rational Design of Chemical Catalysts**
  Robert Harrison (Oak Ridge National Laboratory and University of Tennessee)
- **Next Generation Simulations in Biology: Investigating Biomolecular Structure, Dynamics and Function through Multi-scale Modeling**
  Pratul K. Agarwal (Oak Ridge National Laboratory)
- **Predictive Simulations in Strongly Correlated Electron Systems and Functional Nanostructures**
  Thomas Schulthess (Oak Ridge National Laboratory)

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